

Cross section versus time delay and trapping probability

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Abstract

We study the behavior of the s -wave partial cross section $\sigma(k)$, the Wigner-Smith time delay $\tau(k)$, and the trapping probability $P(k)$ as function of the wave number k . The s -wave central square well is used for concreteness, simplicity, and to elucidate the controversy whether it shows true resonances. It is shown that, except for very sharp structures, the resonance part of the cross section, the trapping probability, and the time delay, reach their local maxima at different values of k . We show numerically that $\tau(k) > 0$ at its local maxima, occurring just before the resonant part of the cross section reaches its local maxima. These results are discussed in the light of the standard definition of resonance.

Keywords: Scattering, Resonances, Square well

PACS: 03.65.Nk, 34.10.+x, 34.50.-s

1. Introduction

By far, the most widely used scattering function is the cross section $\sigma(k)$. Its analysis provides essential information about all kinds of scattering phenomena in physics and it is specially important in the study of resonances. For sharp resonances, the *resonance part* of the cross section is generally assumed to be described by the famous Breit-Wigner resonance formula. Its importance cannot be overestimated since this formula is given in terms of the parameters that characterize the resonance; namely, the width and position of the (cross section) resonance (see e.g. [1] and references therein). This is perhaps the reason why, quite often, the term resonance is taken to mean a resonance in the cross section. In fact, it is sometimes explicitly stated that the resonance energy is defined as that which corresponds to the value of $\pi/2$ of the resonant part of the phase shift, see e.g. [2]. Furthermore, these parameters can be related to some fundamental quantities. For example, in nuclear physics, the width (position) corresponds to the decay width (mass) of a meta-stable particle [3]. Just as knowledge of individual resonances is important, so is the understanding of their statistical properties, such as the distribution of their widths or spacings, specially in the field of quantum chaos [4].

Since the cross section is defined in terms of the phase shift $\theta(k)$ and this is composed of a background part and a resonance part, to unveil the sought after resonance parameters from the data a complicated fitting procedure must be applied [1]. Thus, study of other scattering functions can yield important and complementary information about the system.

The Wigner-Smith delay time $\tau(k)$ [5] is such a quantity. Actually, knowledge of $\tau(k)$ may be considered necessary in order to comply with the most generally accepted definition of resonance [6, 7, 8]. Namely, a rapid increase in the phase shift through $\pi/2$ (modulo π). How fast? Fast enough so that there is time delay since a time delay implies the existence of a meta-stable state and viceversa [8].

In the literature resonances are sometimes defined as the poles of the scattering matrix S [6, 8, 9, 10] (for a more mathematical definition see [11]). We shall refer to these as resonance *poles* to distinguish from the *scattering* resonances discussed above. Certainly, the two definitions are connected and the scattering resonances may be viewed as the manifestation of the resonances poles (occurring near the real axis). However, while the definition of resonance poles is unambiguous, the definition of scattering resonances seems to lack certain consistency that we shall try to point out in the remainder of this paper.

In this paper we shall focus on comparing the behavior of three scattering functions: The s -wave partial cross section $\sigma(k)$,

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the Wigner-Smith time delay $\tau(k)$, and the trapping probability $P(k)$ (to be defined in the next section). We will show that the “speed of the phase shift” $l(k) \equiv 2(\partial\phi/\partial k)$, see Eq. (13) below, can be considered itself a scattering function and it is the link between the other three functions.

One of the objectives of this work is to show that different closely related scattering functions do not in general peak at the same k values as the resonant part of the cross section and hence their study offers complementary information about the resonance properties of the system under study. Although the differences in the peak positions of the various scattering functions may be small there are underlying conceptual differences that may lead to a deeper understanding of resonance phenomena. We shall see that the centers of the resonances of $l(k)$ and $\tau(k)$ can be identified with the real part of the S -matrix poles in k -space, whereas those of $\sigma_\phi(k)$ with the absolute value of the pole.

To be able to get exact results for these quantities we shall use the s -wave central square well potential. Despite the simplicity of this potential, it has served not only as a textbook example to display basic features of quantum resonance scattering [12, 13] but also as a model for some nuclear systems, see e.g. [2, 14, 15, 16]. Paradoxically, some authors have pointed out that the square well does not give rise to “true” non-zero energy resonances [6, 17]. The reason being that precisely at resonances of the cross section, the time delay is at most equal to zero. Others maintain that in spite of this the square well does produce Breit-Wigner resonances, thus advocating the “less restrictive definition of a resonance as an enhancement in the cross section due to a pole in the scattering amplitude” [12]. It appears then that the study of other scattering functions may elucidate the controversy and perhaps induce some polishing in the definition of resonance.

The speed of the phase shift $l(k)$ certainly plays a fundamental role. For the central square well, characterized by the “strength” α (given in Eq. (20)), we demonstrate that the local maxima of $l(k)$ occur just before the resonant part of the cross section reaches its local maxima. Further, we show that $\tau(k) > 0$ at all the local maxima of $l(k)$ except for very large values of α , where $\tau(k) \rightarrow 0$.

2. Scattering functions and resonances

In this brief presentation of the basic scattering quantities, we consider non-relativistic spinless scattering off finite-range potentials. Specifically, potentials decaying as $1/r$ or slower and short range potentials plus a Coulomb-like potentials are not considered here. For central finite-range scattering potentials with free-particle asymptotics, the asymptotic radial wave function ψ_ℓ for the orbital angular momentum l is (see e.g., p. 437 in [8] or p. 6 in [18])

$$\psi_\ell(k; r) = e^{-i\delta_\ell} + S_\ell(k)e^{i\delta_\ell}, \quad r > a_\ell, \quad (1)$$

where a_ℓ is the interaction radius for the ℓ -wave, $\delta_\ell = kr - \ell\pi/2$, $S_\ell(k) = -e^{2i\theta_\ell(k)}$ is the ℓ -wave element of the S -matrix, and

$\theta_\ell(k)$ is the ℓ -wave phase shift. S_ℓ can be written in terms of ψ_ℓ and its space derivative, evaluated at some $r \geq a_\ell$:

$$S_\ell = -e^{-2i\delta_\ell} \frac{1 + ik\psi_\ell/\psi'_\ell}{1 - ik\psi_\ell/\psi'_\ell} \quad (2)$$

$$= -e^{2i\theta_\ell}, \quad (3)$$

where

$$\theta_\ell = -(kr - \ell\pi/2) + \phi_\ell \quad (4)$$

and

$$\phi_\ell = \tan^{-1}[k\psi_\ell(k; r)/\psi'_\ell(k; r)] \quad (5)$$

is the so-called resonant part of the phase shift. Clearly, the phase shift $\theta_\ell(k)$ is independent of the radius r as long as it is in the asymptotic regime ($r \geq a$, where a is the interaction radius), whereas the resonant part $\phi_\ell(k)$ depends on the radius $r \geq a$ where it is calculated. For well defined radius of interaction a the natural choice for the evaluation of ϕ is $r = a_\ell$, see also Ref. [15].

2.1. Cross section

As shown in most books on quantum mechanics, for central potentials the s -wave partial cross section is given by

$$\sigma_\ell(k) = \frac{4\pi(2\ell+1)}{k^2} \sin^2(\theta_\ell). \quad (6)$$

In this work we shall consider only the case $\ell = 0$; s wave scattering. Dropping the subscript $\ell = 0$ in all quantities, the s partial wave cross section is then written as

$$\sigma(k) = \frac{4\pi}{k^2} \sin^2(\theta) = \frac{\pi}{k^2} |1 + S|^2, \quad (7)$$

where $S = -\exp(2i\theta)$, k is the wave number in the asymptotic region, and $\theta(k) = -kr + \phi$. Clearly, the phase shift $\theta(k)$ is independent of the radius r as long as it is in the asymptotic regime ($r \geq a$, where a is the interaction radius), whereas the resonant part ϕ depends on the radius $r \geq a$ where it is calculated. For s -waves, if $r = a$, the phase $-ka$ is the so-called hard sphere shift. As is customary [19] and convenient for our purposes, we shall be considering the scaled version of the cross section (or scattering amplitude):

$$\sigma_\theta(k) = \frac{k^2}{\pi} \sigma(k) = |1 + S|^2 = 4 \sin^2(\theta) \quad (8)$$

and its resonance part

$$\sigma_\phi(k) = 4 \sin^2(\phi). \quad (9)$$

An important reason to separate the phase shift into resonant and non resonant parts is that the resonance formula of Breit-Wigner refers exactly to the resonant part of the phase shift. Since this is not the usual case, there are formulas, like that of Fano’s resonance shape [20] that can be used to fit and extract the so-called Breit-Wigner parameters defining the center and the width of the resonance [18, 21]. These parameters, in the relativistic case, provide the (Breit-Wigner) mass and life time of the unstable particles. As far as we know [1] this requires fitting procedures with often several fitting parameters. The point is that in many practical applications, the splitting of the phase shift is needed to make sense of the data.

2.2. Time delay and effective traversal distance

The time delay is a commonly used quantity to characterize resonances, see e.g. [6, 7, 18, 22]. In one dimension it is known also as the Wigner-Smith time delay and for a particle of mass μ with incident momentum $\hbar k$, it is defined as [23, 24]

$$\tau(k) = -i\hbar S^* \frac{\partial S}{\partial E} = 2\hbar \frac{\partial \theta}{\partial E} \quad (10)$$

$$= \frac{\mu}{\hbar k} 2 \frac{\partial \theta}{\partial k}. \quad (11)$$

It is the difference between the time that a particle spends in the internal region in the presence of a scattering potential minus the time the particle would spend if there were no scattering potential [25]. $\tau(k)$ is directly connected with the existence of meta-stable states or the temporary capture of the projectile in the interaction region [8]. As mentioned in the Introduction, the established definition of resonance requires that $\tau(k)$ be greater than zero. The quantity $2(\partial\theta/\partial k)$ was called the “retardation stretch” by Wigner [23]. He used it to derive his causality condition, discussed in most books on scattering theory (see e.g. page 103 in [22] or page 466 in [8]). By splitting the phase shift into resonant and non-resonant parts (10) becomes

$$\tau(k) = \frac{\mu}{\hbar k} [l(k) - 2a], \quad (12)$$

where

$$l(k) \equiv 2 \frac{\partial \phi}{\partial k}. \quad (13)$$

In contrast with the retardation stretch, the quantity $l(k)$ is the change with k of the purely resonant part of the phase ϕ . We shall refer to $l(k)$ as the speed of the resonant part of the phase shift, or, briefly speed of the phase shift. In the case of scattering off finite range potentials with a radius of interaction a , the interpretation of $\tau(k)$ as time delay leads us to interpret $l(k)$ as the distance a particle would travel under the action of the potential but with constant momentum $\hbar k$. That is, an *effective traversal distance*. Note that even though $\tau(k)$ and $l(k)$ are defined in terms of the asymptotic quantities θ and ϕ , respectively, they give information about the time spent and effective traversal distance within the interaction region.

2.3. Trapping probability

For a localized potential with radius of interaction a the quantity

$$P(k) \equiv \frac{1}{a} \int_{int} |\psi(k; r)|^2 dr, \quad (14)$$

gives the relative probability of trapping or dwelling in the interaction region. Here, $\psi(k; r)$ is the scattering wavefunction. The denominator a in the definition of $P(k)$ implies normalization with respect to a scattering state with uniform density $|\psi(k; r)|^2 = 1$ within the interaction region. Although the normalization is arbitrary, what is important is the behavior of P as a function of k . It can be shown that $P(k)$ can be represented alternatively as

$$P(k) = \sum_{\lambda} |A_{\lambda}^B(k)|^2. \quad (15)$$

Here A_{λ}^B , $\lambda = 1, 2, 3..$ are the coefficients in the expansion of $\psi(k; r)$ within the internal region ($0 \leq r \leq a$) in terms of a complete set of (reaction) states $\Phi_{B,\lambda}$ defined in the reaction matrix theory of Wigner [26] (see also e.g. [2, 18, 27, 28]). In the reaction matrix theory, the configuration space is divided in two regions; the internal or reaction region ($0 \leq r \leq a$) and the asymptotic region $r \geq a$. B is the boundary value parameter specifying the logarithmic derivative obeyed by the set $\{\Phi_{B,\lambda}, \lambda = 1, 2, \dots\}$.

In order to show the relation between $\sigma_{\phi}(k)$, $P(k)$ and $\tau(k)$, it is convenient to write the tangent of (5) as $\tan(\phi) = kR_0$, where $R_0 \equiv \psi_{\ell}(k; r)/\psi'_{\ell}(k; r)$. R_0 is the so-called reaction function corresponding to the boundary value parameter equal to zero [27]. It is straightforward to see that

$$l(k) = \frac{2(R_0 + kR'_0)}{1 + (kR_0)^2}, \quad R'_0 \equiv \frac{\partial R_0}{\partial k}. \quad (16)$$

It can also be shown, by expressing the expansion coefficients A_{λ}^B in terms of R_0 , that

$$aP = 2 \frac{kR'_0}{1 + (kR_0)^2}. \quad (17)$$

Comparing (16) with (17) and writing back R_0 in terms of ϕ gives

$$aP = l(k) - \frac{\sin(2\phi)}{k}. \quad (18)$$

This, together with (12) gives the relation between $P(k)$, $\tau(k)$ and $l(k)$. Expressions (16) to (18) are true for all central potentials as long the potential can be considered negligible for some $r > a$.

3. Application to the central square well

3.1. Expressions

The potential is $-|V_0|$ in $0 < r < a$ and zero everywhere else. The wave number q in the internal region is related to the wave number k in the external region by

$$q^2 a^2 = \frac{2\mu a^2}{\hbar^2} (E + |V_0|) = k^2 a^2 + \alpha^2, \quad (19)$$

with

$$\alpha^2 \equiv \frac{2\mu a^2}{\hbar^2} |V_0|. \quad (20)$$

The wave function in the internal region is

$$\psi(k, r) = A \sin(qr), \quad 0 \leq r \leq a, \quad (21)$$

where

$$A = -2i \frac{(k/q) e^{-ika}}{\cos(qa) - i(k/q) \sin(qa)}. \quad (22)$$

The wave function outside the well is

$$\psi(k, r) = e^{-ikr} + S e^{ikr}. \quad (23)$$

By means of the continuity of the wave function, c.f. (21) and (23) at $r = a$, it follows that

$$S = -e^{-2ika} \frac{\cos(qa) + i(k/q) \sin(qa)}{\cos(qa) - i(k/q) \sin(qa)} \quad (24)$$

$$= -e^{2i\theta}, \quad (25)$$

where

$$\theta = -ka + \phi \quad (26)$$

and the resonant part of the phase shift ϕ is given by

$$\tan(\phi) = k \frac{\tan(qa)}{q}. \quad (27)$$

That is, for the square well, the background phase shift is $-ka$, the so-called hard sphere phase shift. It follows from (23) that the probability $|\psi(k; a)|^2$ of finding the particle at the boundary between the internal and external regions is equal to $\sigma_\phi(k)$:

$$|\psi(k; a)|^2 = 4 \sin^2(\phi) = \sigma_\phi(k). \quad (28)$$

This equation shows that it is ϕ , not θ , that completely determines the coupling of the internal system with the projectile. $\sigma_\phi(k)$ can be expressed in terms of the amplitude A of the wave function inside the well using continuity of the wave function at $r = a$ with (21) and (28):

$$\sigma_\phi(k) = |A|^2 \sin^2(qa), \quad (29)$$

where, c.f. (22),

$$|A|^2 = \frac{4(ka)^2}{(ka)^2 + \alpha^2 \cos^2(qa)}. \quad (30)$$

Similarly, using (21) into (14) and integrating, $P(k)$ can be written as

$$P(k) = \frac{|A|^2}{2} \left(1 - \frac{\sin(2qa)}{2qa} \right). \quad (31)$$

It can be verified that this expression can be obtained from the more general results: (17) or (18).

Now let us consider $\tau(k)$. The background shift phase is $-ka$. Hence equation (12) becomes

$$\tau(k) = \frac{\mu}{\hbar k} (l(k) - 2a). \quad (32)$$

After a little algebra using, for example, (18) and (31) $l(k)$ can be written as

$$\frac{l(k)}{2a} = \frac{|A|^2}{4} \left(1 + \frac{2|V_0| \sin(2qa)}{k^2} \right) \quad (33)$$

$$= \frac{P(k)}{2} + \frac{1}{2} \frac{qa \sin 2qa}{(ka)^2 + \alpha^2 \cos^2(qa)}. \quad (34)$$

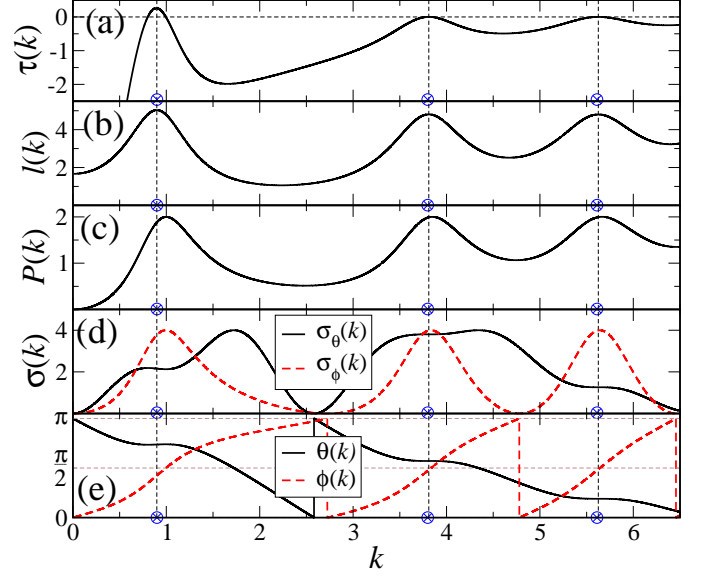


Figure 1: (Color online) Scattering functions for rectangular Well I: $a = 2.4$, $V_0 = -10$, and $\alpha = 10.733$. (a) $\tau(k)$, (b) $l(k)$, (c) $P(k)$, (d) $\sigma(k)$ ($\sigma_\phi(k)$ and $\sigma_\theta(k)$), and (e) the phases $\theta(k)$ and $\phi(k)$. The vertical dashed lines indicate the positions of the local maxima of $l(k)$. The encircled crosses mark the positions of the real part k_n of the poles of the S -matrix in complex k -space.

3.2. Results

The first result is implied by (32). It tells us how fast the resonant part of the phase shift must increase in order for meta-stable states to exist. The condition is $l(k) > 2a$.

Several authors have obtained approximate expressions for $\tau(k)$ at the local maxima of $\sigma_\phi(k)$, i.e. at $\phi = \pi/2$ modulo $\pi/2$, to show that for the square well the resonant part of the phase shift increases as fast as the background ($-ka$) decreases. Therefore there is no time delay and consequently, according to the established definition of resonance, the local maxima of $\sigma_\phi(k)$ are not true resonances, see e.g. [6, 17]. Here, (33) together with (30) show without approximations that indeed $l(k) = 2a$ at $qa = \pi/2$ modulo π (equivalently, $\phi = \pi/2$ modulo π) and hence $\tau(k)$ is exactly zero at the local maxima of $\sigma_\phi(k)$. However, as we shall show below, $l(k) \geq 2a$ at its own local maxima, which occur very nearly where the local maxima of $\tau(k)$ occurs.

We shall first consider in detail four rectangular wells, specified by their width and depth, listed in the second column of Table 1. The reasons for choosing these particular parameter values will be clear below.

In Fig. 1 we plot the scattering functions $\tau(k)$, $l(k)$, $P(k)$, $\sigma_\theta(k)$, and $\sigma_\phi(k)$ for Well I. In the lowest panel we show ϕ and θ , modulo π . In these figures we also mark with an encircled cross the positions of the real value of the S -matrix pole in k -space. These poles were calculated numerically by finding the complex zeroes of the denominator of A (22). Further, the peaks of $l(k)$ are marked with vertical dashed lines. It is evident that not all scattering functions reach their local maxima at the same k value. Let us label the position of the n^{th} peak of $l(k)$, $\tau(k)$, $P(k)$, and $\sigma_\phi(k)$ by k_n^* , k_n^τ , k_n^P , and k_n^s , respectively.

Let us comment on the following features shown in Fig. 1:

Well	$a, V_0 $	α	Q_B	k_1^*	k_1^τ	k_1^P	k_1^σ	κ_1	$ K_1 $	$l(k_1^*)/2a$
I	2.4, 10	10.733	3.91	0.8983	0.8934	0.9990	0.9950	0.8994	0.9936	1.0486
II	12, 10	53.665	17.58	0.9915	0.9915	0.9952	0.9950	0.9913	0.9949	1.0014
III	12, 10/25	10.733	3.91	0.1797	0.1787	0.1990	0.1990	0.1799	0.1987	1.0486
IV	8.7326, 10	39.0535	12.931	0.4572	0.4570	0.4716	0.4714	0.4572	0.4714	1.0153
V	8.7766, 10	39.2505	12.994	0.0585	0	0.1407	0.1406	0.0825	0.1407	1.352
VI	8.7546, 10	39.1520	12.962	0.3274	0.3269	0.3475	0.3474	0.3279	0.3473	1.0293
VII	8.7987, 10	39.3489	13.025	1.7948	1.7948	1.7991	1.7985	1.7943	1.7983	1.0009

Table 1: Parameters and scattering properties for seven representative wells. The values of ϕ at the first local maximum of $l(k)$ are: 1.33, 1.53, 1.33, 0.68, 1.39, 1.44, and 1.54 for Wells I to VII, respectively.

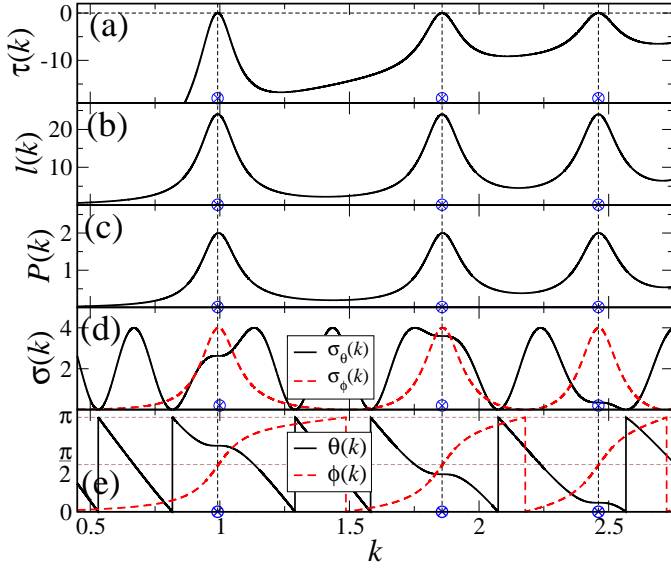


Figure 2: (Color online) Scattering functions for the rectangular Well II: $a = 12$, $V_0 = -10$, and $\alpha = 53.665$. Same description as in Fig. 1.

1. The peaks of both, $l(k)$ and $\tau(k)$ seem to coincide exactly with the real part κ_n of the n^{th} resonance S -matrix pole in k -space. How close these are to each other can be seen by comparing the first row in Table 1; columns 5 and 6 with column 9. The percentual difference between k_1^* and κ_1 is about 0.1, and between k_1^τ and κ_1 is a little larger, about 0.6.
2. The centers of the local maxima of $\sigma_\phi(k)$ occur, very close to $|K_1|$, the absolute value of the pole in k -space. Compare columns 8 and 10, first row, Table 1. The percentual difference is about 0.1. This may be surprising, since it is usually assumed, via the Breit-Wigner formula, that the centers of the $\sigma_\phi(k)$ peaks correspond to the real part of the S -poles in energy space. This finding is complementary to that of Klaiman and Moiseyev [29] who showed numerically and analytically that the transmission resonances for 1D potentials (that is 2 channels, instead of one channel as is our case) occur at $|K_n|^2/2$ rather than at its real part E_R .

It can be shown analytically, using a one-level model in

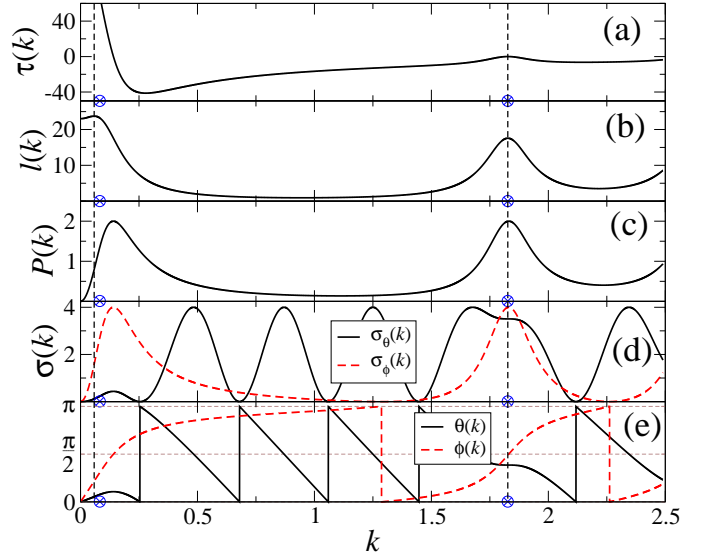


Figure 3: (Color online) Scattering quantities for the rectangular Well V: $a = 8.7766$, $V_0 = -10$, and $\alpha = 39.2505$. Same description as in Fig. 1.

- reaction matrix theory, that indeed $k_n^* \approx k_n^\tau \approx \kappa_n$ and $k_n^S \approx |K_n|$. The proof of these results, valid for all localized central scattering potentials, will be published elsewhere.
3. The first peak of $P(k)$ seems to occur exactly where $\sigma_\phi(k)$ peaks (of course, at $\phi = \pi/2$ modulo π). Table 1 shows that actually $k_1^P - k_1^S = 0.004$. The difference $k_n^P - k_n^S > 0$ becomes noticeable for the second local maxima ($n = 2$) and it increases with n . This pattern can be understood by examining (31) to (32) and noticing that all the local maxima of both, $\sigma_\phi(k)$ and k^S , are the same as those of $|A|^2$ but different from those of $P(k)$ because of the term $f = 1 - \sin^2(qa)/(qa)$. For k_n^P to be close to k_n^S , the term f must be close to one. Equation (31) shows this occurs for $\alpha \gg 1$ (α of the order of 30 is sufficient) but also for intermediate values of α (say, 10) but for $ka < 10$. In contrast, for α of the order of one or less, the term f makes $P(k)$ to be drastically different from $|A|^2$. Hence, the behavior as a function of k of the trapping probability and the relative intensity (or probability) $|A|^2$ in the interior of the well are very similar quantitatively only for very strong potentials ($\alpha \gg 1$) or for intermediate values

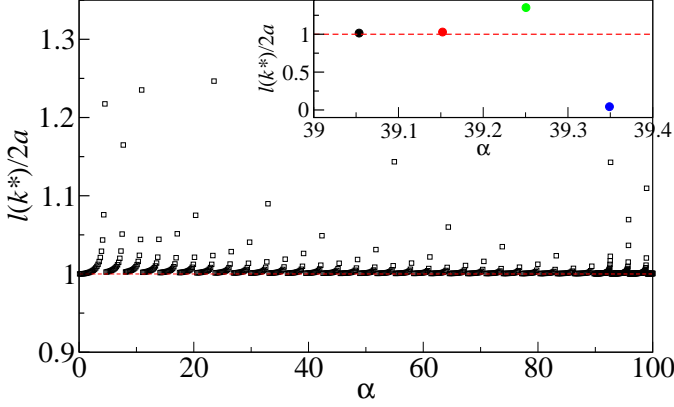


Figure 4: (Color online) First local maxima of $l(k)$ as a function of α . Inset: Details for Wells IV, V, VII, and VII; see Table 1.

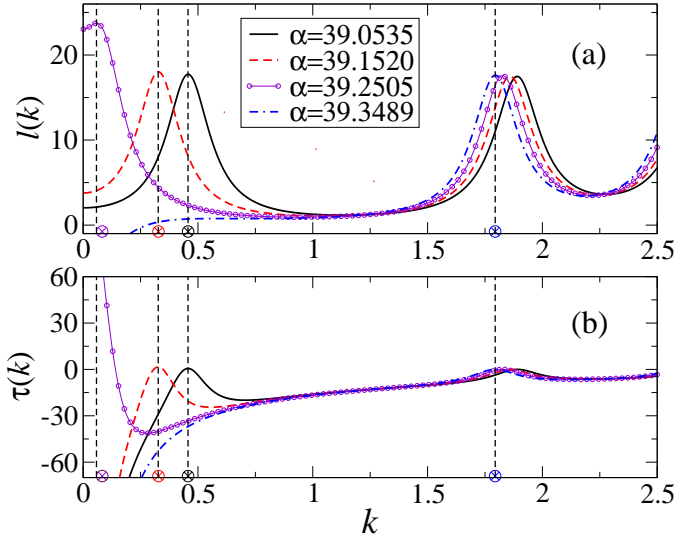


Figure 5: (Color online) (a) Effective traversal length $l(k)$ and (b) time delay $\tau(k)$ for rectangular Wells IV, V, VI, and VII.

of α but with $ka < \alpha$.

4. In panel (a) we see that both, $\tau(k)$ and $l(k)$ peak apparently at $k = \kappa_1$ and $\tau(k) > 0$ in a small neighborhood of it. This is remarkable given that in panel (d) the full phase θ looks pretty flat. As we showed above $\tau(k)$ is exactly zero at $\phi = \pi/2$ (modulo π). However, there is a small positive slope, just before $\phi = \pi/2$. It is small but sufficiently large to make $l(k) > 2a$ (see last column of Table 1) and hence produce a time delay. This positive slope has been reported previously [17] but the authors dismiss by claiming that, in an approximation valid for α very large, it cannot create a Breit-Wigner resonance. Here we see that it can be considered as a true resonance because the phase shift changes fast enough to produce a time delay and, although its maximum does not occur at $\phi = \pi/2$, it goes through $\pi/2$ during resonance. Moreover, there is clearly a resonance pole associated with the maximum change in the phase shift and it is responsible too for the Breit-Wigner like behavior of $P(k)$ and $\sigma_\phi(k)$.

We shall determine below under what conditions $\tau(k)$ is greater than zero at its local maxima.

5. The plot of the reduced cross section $\sigma_\theta(k)$ illustrates how the background phase shift hides the pure resonance structure evidenced by $\sigma_\phi(k)$. The effect of the background in the cross section is well known, see e.g. [6, 8, 18]. For sharp resonances, the effect of the background is studied by writing $\sigma_\theta(k)$ in terms of the Fano profile parameter. For not so sharp resonances, complicated algorithms must be used and the results are model dependent, as is the case in nuclear scattering phenomena [1, 9, 30].

Figure 2 plots the scattering functions of square Well II. It is 5 times wider than Well I; correspondingly, the “strength” α is 5 times larger. The resonance structure is sharper than for the Well I because as α increases the relative intensity $|A|^2$ has sharper and deeper oscillations, see (30). The effect is the same for all scattering functions since they all have the prefactor $|A|^2$ in common. The features displayed by this well are qualitatively similar to those of square Well I except that now the peaks of $\tau(k)$ and $l(k)$ move closer to $\phi = \pi/2$. We see that as the resonances become sharper the position of the peaks of all these scattering functions seem to converge to $k = \kappa_n$, as suggested by Fig. 2. Another distinctive feature is that $\tau(k)$ is now barely larger than zero at its peak. Correspondingly, $l(k)$ has increased by about five times but is barely larger than $2a$, see last column of Table 1.

Consider the Well II listed in Table 1. It has different width and depth but shares with Well I the value of α . It can be seen from (27) that ϕ depends on the adimensional variable ka (or qa). Then for any two wells with the same α , the phase $\phi(k)$ corresponding to a well of width a will be the same as the phase $\phi(k')$ corresponding to a well of width a' if $ka/a' = k'$. Hence, the plots for $P(k)$ and $\sigma_\phi(k)$ will be the same but the k -axis multiplied by a factor of a/a' . The same for $l(k)$ and $\tau(k)$, but in addition, $l(k)$ and $\tau(k)$ will now be divided by the same factor since these two quantities involve the derivative with respect to k . The data obtained for Well III in Table 1 confirms this scaling. Note that the centers of the peaks and the poles themselves are scaled by 5 and the peak of the effective traversal length $l(k^*)$ divided by $2a$ is the same for both wells. Here, k^* are the values for which $l(k)$ is a local maxima.

Often one finds in the literature approximations or statements made for deep potentials. The abovementioned scaling emphasizes that the more relevant quantity is α (20), and not just the depth. A peculiarity of the square well is that the value of α determines the number of bound states and hence, very strongly, the scattering properties for the low lying resonances. We have found that a very good approximation for the number N_B of bound states is given by the integer part of [31]

$$Q_B = (\alpha/\pi + 1/2), \quad (35)$$

In column 4 of Table 1, we list Q_B for all wells considered here. The formula predicts that there are 3 bound states for Wells I and III, 17 bound states for Well II, 12 for Well IV, and so on. Moreover, the fractional part of Q_B indicates us how

close the bound state is to the continuum. In other words, it indicates how close it is to fit the next bound state. Let us skip momentarily Well IV and consider Well V listed in Table 1; Well V has $\alpha = 39.2505$ and its scattering functions are plotted in Fig. 3. According to our interpretation above, Well V (with $Q_B = 12.994$) is almost strong enough to bind 13 states. I.e., the 13th state corresponds to the first scattering resonance close to $k = 0$. The predictions based on the interpretation of formula (35) have been verified numerically. We shall now see how critically the fractional part of Q_B determines the scattering properties of the well.

Notice that the real part of the first resonance pole for Well V (II) is the smallest (largest) of the first five wells and how this reflects in the scattering properties displayed in Figs. 1 to 3. Focusing on Well V, Fig. 3, we see that now the first resonance of all its scattering functions come closer to $k = 0$ as predicted above. We also note that the resonance profiles have changed drastically. The bell-like shape of $\sigma_\phi(k)$ and of $P(k)$ have become skewed and become zero at $k = 0$. Now the maxima of $l(k)$ is significantly larger than $2a$ but has lost its bell shape profile. Moreover $\tau(k) \rightarrow \infty$ as $k \rightarrow 0$.

We can understand this behavior by examining the formulas (31) to (34). These show that $|A|^2 \rightarrow 0$ and $P(k)$ clearly zero at $k = 0$. Further $l(k)/(2a)$ equals $(qa/\alpha^2) \tan(qa)$. Note also that now the local maxima of $\sigma_\phi(k)$, $P(k)$, and even $l(k)$, are more distant now from the real part of the S -matrix pole. This feature, discussed in a future publication, can be understood by means of reaction matrix theory.

The resonance pattern displayed by Well V pertains to very low energy resonances, not the case of the so-called zero energy resonances where the s -wave scattering cross section (7) becomes infinite, see e.g. [6, 7, 8, 17].

Now we want to show numerically that all resonances of $l(k)$ and $\tau(k)$ yield a positive time delay. Perhaps “positive time delay” seems redundant for if there is a time delay, it must be positive. However, since time delay is already the name of the function and it can be zero or negative, we add the adjective positive. Figure 4 shows the *first* maxima of $l(k)/(2a)$ as a function of α . Recall that k^* are the values for which $l(k)$ is a local maxima. Inspection of this plot and its data shows that all first maxima $l(k^*)$ are larger or equal to $2a$, hence $\tau(k^*)$ is greater than zero. Notice the periodic monotonic increase of $l(k^*)/(2a)$ as α increases and then drops back to $l(k^*)/(2a) \approx 1$. In the inset of Fig. 4 we zoom on four consecutive first maxima of $l(k)$, corresponding to 4 wells varying slightly in their values of α . These four wells are labeled IV, V, VI, and VII in Table 1. Wells IV, V, and VI, with $\alpha = 39.0535$, 39.1520 , and 39.2505 , respectively, have 12 bound states according to the integer value of their Q_B . By the same token, Well VII has 13 bound states. The effective traversal distance and the time delay of these four wells are plotted in Fig. 5. Figure 5 exemplifies the pattern observed in Fig. 4; namely, as α increases an additional state is bound; the closer the first resonance state is to $k = 0$, the larger the time delay. Simultaneously, the value of the resonant part of the phase shift ϕ moves down away from $\pi/2$ (see Table 1). Conversely, as the first maxima of $l(k)$ moves up away from $k = 0$ the phase ϕ at the local maxima of $l(k)$ becomes closer to

$\pi/2$. The larger α is, the sharper the resonances are and at the same time the closer these occur to $\pi/2$. We have shown that $\tau(k) = 0$ exactly at $\phi = \pi/2$. This is perhaps the reason why in previous studies, which assume very large values of α no time delays have been observed.

4. Conclusions

The reason for requiring, in the established definition of a scattering resonance, a rapid increase in the total phase shift θ comes from the idea that a “true” resonance is to correspond to the formation of a meta-stable state or to the temporary trapping of the projectile in the scattering region (see e.g. [6, 7, 22]). Trapping leads to a time delay of the scattered wave, which in turn implies that the Wigner-Smith time delay $\tau(k)$ must be positive.

Our expressions shows that for $\tau(k)$ to be greater than zero, the effective traversal distance $l(k)$ must be greater than twice the width of the well. We demonstrated numerically that this is so for the square well for all the local maxima of $\tau(k)$. Moreover, we showed numerically that the peaks of $\tau(k)$ and $l(k)$ occur very close to each other and to the real part of the S -matrix resonance poles. We also showed that although the peaks of $\tau(k)$ occur for values of ϕ slightly smaller than $\pi/2$ (modulo π), ϕ jumps by about π from beginning to end of the resonance passing through $\pi/2$. So, it meets the requirements of the established definition of resonance, except that the peak of $\tau(k)$ does not occur exactly at $\pi/2$, where the resonant part of the scattering cross section reaches its unitary limit. On the other hand, we showed that as α becomes large, the local maxima of $\tau(k)$ and $l(k)$ occur closer to $\phi = \pi/2$ (modulo π). Simultaneously $l(k) \rightarrow 2a$ and consequently $\tau(k) \rightarrow 0$. This explains why most studies on the resonances properties of the square well, which focus on large values of the “strength” α (usually referred to as deep potentials), arrive at the conclusion that the square well does not produce meta-stable states.

The study of this simple system leads us to question about the conventional or popular definition of scattering resonances. Specifically, it raises the question about how essential is it that the time delay be positive exactly at $\pi/2$ for it to be true scattering resonance? Why is the cross section and not other scattering function, like the dwelling time, or the trapping probability be the standard or preferred scattering function to define a scattering resonance? After all, time delay $\tau(k)$, trapping probability $P(k)$, relative intensity $|A|^2$, and cross section $\sigma(k)$ are all aspects of the same scattering phenomena and these are expected to display similar behavior under resonance. $P(k)$ and $\sigma(k)$ have more in common with each other than with $\tau(k)$ and $l(k)$. The first pair relate to probabilities while the last pair relate to changes. So, it appears that the information they carry is complementary.

The quantum mechanical definition ultimately originates from the classical definition of scattering cross section. Is this the main reason why even popular text books in quantum mechanics at graduate level define scattering purely in terms of the cross section?

We believe these questions have not been raised, or at least, as far as we know, have not been published, because most studies of resonances deal with sufficiently sharp resonances, for which, as we have seen, time delay, and cross section coincide in their peaks. In fact, it is well known that both, the cross section and the time delay, are proportional to each other and are described by the Breit-Wigner resonance formula. This of course is an approximation, valid for sharp resonances, or equivalently for resonance poles near the real axis where a one-pole approximation lead to the Breit-Wigner formula. The center of the resonance is usually associated with the real part of the pole in energy space. Our numerical studies show, however, that it is more closely related to the absolute value of the resonance pole (in energy or wave number space).

It is natural to ask if the scattering properties presented here for the central square well are expected to be true also for more general or realistic finite-range potentials. The main results rely on the separation of the phase shift into the hard-sphere phase shift $-ka$ and resonance part ϕ . If the radius of interaction a is well known, then the choice $r = a$ is the optimum choice. If a is only known approximately or the evaluation (measurement) of the phase shift can be done only for a radius $r > a$ then it is necessary to examine how the scattering quantities $\tau(k)$, $l(k)$, $P(k)$ and $\sigma_\phi(k)$ change with changes of r (in the asymptotic region). First we note that the full phase shift θ does not depend on $r \geq a$. Thus, the time delay, which is ultimately defined in terms of θ , does not depend on $r \geq a$ either. The same is true for the scattering cross section $\sigma_\theta(k)$.

For the speed of the phase shift $l(k)$ let us consider two arbitrary radius of separation (r_1 and r_2) for the resonant part ϕ ; $\phi_1 = \theta + kr_1$ and $\phi_2 = \theta + kr_2$. Since θ is independent of the radius r , it follows that $\phi_2 = \phi_1 + k(r_2 - r_1)$; hence $l_2(k) = l_1(k) + (r_2 - r_1)$. Thus these two differ by the constant $r_2 - r_1$. Hence the shape of $l(k)$ evaluated at some $r \geq a$ is the same (except higher by a distance $r - a$) as if evaluated at the radius of interaction a . Moreover, the centers of their local maxima occur at the same value of k . This result is independent of the potential, as long as it has a finite range. Further, for the central square well we showed numerically that the n^{th} local maxima of $l(k)$ occur in a very small neighborhood of κ_n , the real part of the pole in complex k -space. Work in progress suggests strongly that this feature is true for any finite-range potential.

This property is not shared by the trapping probability. Consider the integrals $P_a = \int_0^a |\psi(k; r)|^2 dr$ and $P_r = \int_0^r |\psi(k; r)|^2 dr$, corresponding, respectively, to radii a , the actual radius of interaction, and $r > a$. It can be easily shown that $P_r = (a/r)P_a + 2(r - a)/r - [\sin(2\phi_r) - \sin(2\phi_a)]/kr$, where ϕ_r and ϕ_a are the resonant part of the phase shift evaluated at radius $r > a$ and a , respectively. This shows that the profiles of P_a and P_r as a function of k can be very different if $r - a$ is not very small or k is not very large. In such case, the centers of their peaks will be very different too. On the other hand, Figs. 1-3, for the central square well, show that when $r = a$ the trapping probability $P_a(k)$ under resonance conditions assumes a lorentzian-like shape, similar to the shape of the other scattering quantities. If this lorentzian shape were to be universal for all short-range potentials, then it can be used as a criteria to determine the radius of interac-

tions. Work in progress carried out in a variety of short-range potentials indicates that indeed this shape is universal.

This universality is not obeyed for the purely resonant scattering cross section $\sigma_\phi(k)$. In fact, even for the central square well, different values of r used in the evaluation of the resonant phase ϕ can produce shapes of $\sigma_\phi(k)$ that differ radically from the well known Breit-Wigner resonance formula, attained when $r = a$. However, this may not be seen as a negative quality for it serves to discriminate between the actual radius of interaction and other radii and is consistent with the behavior of the trapping probability.

Thus, while not all features presented by the central square well can be generalized to arbitrary potentials, the merit of the square well is that it reveals subtle but important distinctions between the various scattering functions that motivates their study in more realistic systems.

Acknowledgments. This work was partially supported by Fondo Institucional PIFCA (Grant No. BUAP-CA-169). J.A.M.-B thanks support from CONACyT (Grant No. CB-2013/220624) and VIEP-BUAP (Grant No. MEBJ-EXC14-I). A.A.F.-M. thanks financial support from DGAPA-UNAM.

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